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(FILE 'HOME' ENTERED AT 08:24:10 ON 14 OCT 2004)

FILE 'CASREACT' ENTERED AT 08:26:21 ON 14 OCT 2004

L1 STRUCTURE UPLOADED  
L2 0 S L1  
L3 1 S L1 FUL  
L4 STRUCTURE UPLOADED  
L5 0 S L4  
L6 1 S L4 FUL

FILE 'CAPLUS' ENTERED AT 08:35:44 ON 14 OCT 2004

L7 389101 S COUPLING  
L8 1570 S ARYL BROMIDE#  
L9 4345 S ARYL HALIDE#  
L10 5458 S L8 OR L9  
L11 198737 S KETONE#  
L12 389101 S L7  
L13 140 S L7 AND L10 AND L11  
L14 143277 S PALLADIUM  
L15 82 S L14 AND L13  
L16 5173 S BRONSTED  
L17 614351 S BRONSTED OR BASE  
L18 15 S L17 AND L15

=> d bib abs kwic 1-15

L18 ANSWER 1 OF 15 CAPLUS COPYRIGHT 2004 ACS on STN  
AN 2004:218750 CAPLUS

DN 140:253348

TI Preparation of biaryls from **aryl halides** and  
arylboranes

IN Nishida, Mayumi; Tagata, Takeshi

PA Koei Chemical Co., Ltd., Japan

SO Jpn. Kokai Tokkyo Koho, 16 pp.

CODEN: JKXXAF

DT Patent

LA Japanese

FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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PI JP 2004083530	A2	20040318	JP 2002-249649	20020828
PRAI JP 2002-249649		20020828		

OS MARPAT 140:253348

AB Biaryls are prepared by reaction of **aryl halides** with  
arylboronic acids or dialkylarylboranes in solvents in the presence of (a)  
Pd catalysts, which are insol. in solvents and show specific x-ray  
photoelectron spectra, (b) bases, and (c) phosphines. P-ClC<sub>6</sub>H<sub>4</sub>CN was  
treated with PhB(OH)<sub>2</sub> in 1,2-dimethoxyethane in the presence of PPh<sub>3</sub>,  
KHCO<sub>3</sub>, and Pd/C at 80° for 8 h to give 67% 4-cyanobiphenyl.

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KHCO<sub>3</sub>, and Pd/C at 80° for 8 h to give 67% 4-cyanobiphenyl.

ST biaryl prepn **aryl halide coupling**  
arylborane; **palladium catalyst aryl halide**  
**coupling** arylborane; phosphine base palladium

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L3 1 S L1 FUL

=> d bib abs crd 13

L3 ANSWER 1 OF 1 CASREACT COPYRIGHT 2004 ACS on STN

AN 108:94141 CASREACT

TI 2-Ethynylbenzenealkanamines. A new class of calcium entry blockers  
AU Carson, J. R.; Almond, H. R.; Brannan, M. D.; Carmosin, R. J.; Flaim, S.  
F.; Gill, A.; Gleason, M. M.; Keely, S. L.; Ludovici, D. W.; et al.

CS McNeil Pharm., Spring House, PA, 19477-0776, USA

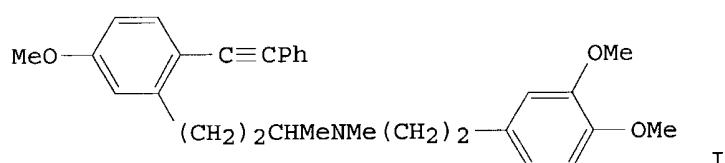
SO Journal of Medicinal Chemistry (1988), 31(3), 630-6

CODEN: JMCMAR; ISSN: 0022-2623

DT Journal

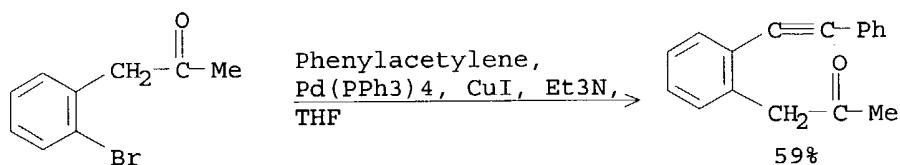
LA English

GI



AB A series of 2-[aryl(alkyl)ethynyl]benzenealkanamines was synthesized. The compds. exhibit antihypertensive activity in spontaneously hypertensive rats and coronary vasodilator activity with minimal neg. inotropic activity in the Langendorff guinea pig heart in vitro. They exert their activity by inhibition of Ca<sup>2+</sup> influx across cell membranes. Optimal activity is found among the N-(arylethyl)-5-methoxy- $\alpha$ -methyl-2-(phenylethyynyl)benzeneethanamines and -propanamines, e.g., I.

RX(25) OF 149



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(FILE 'HOME' ENTERED AT 08:24:10 ON 14 OCT 2004)

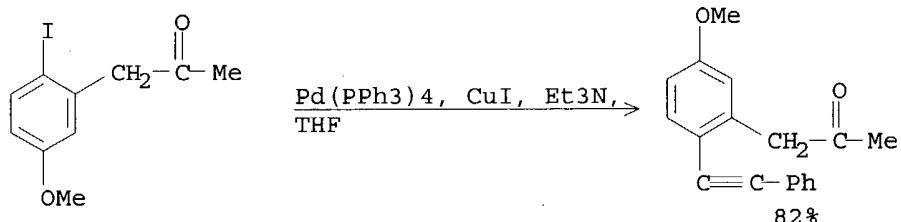
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L2                0 S L1  
L3                1 S L1 FUL  
L4                   STRUCTURE UPLOADED  
L5                0 S L4  
L6                1 S L4 FUL

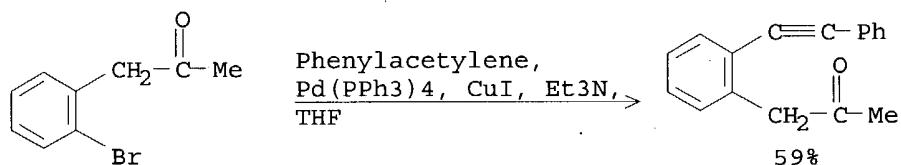
=> d crd bib

L6   ANSWER 1 OF 1    CASREACT   COPYRIGHT 2004 ACS on STN

RX(3) OF 149



RX(25) OF 149



AN 108:94141 CASREACT

TI 2-Ethynylbenzenealkanamines. A new class of calcium entry blockers  
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DT Journal

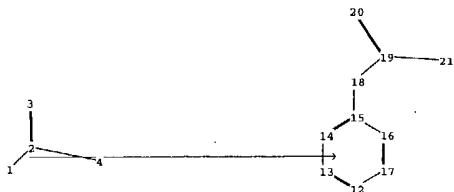
LA English

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Pd



24



chain nodes :  
1 2 3 11 18 19 20 24

ring nodes :

5 6 7 8 9 10 12 13 14 15 16 17

ring/chain nodes :

4 21

chain bonds :

1-2 2-3 2-4 8-11 15-18 18-19 19-20 19-21

ring bonds :

5-6 5-10 6-7 7-8 8-9 9-10 12-13 12-17 13-14 14-15 15-16 16-17

xact/norm bonds :

2-3 19-20

xact bonds :

1-2 2-4 8-11 15-18 18-19 19-21

normalized bonds :

5-6 5-10 6-7 7-8 8-9 9-10 12-13 12-17 13-14 14-15 15-16 16-17

catch level :

1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom  
11:CLASS 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:CLASS 19:CLASS

20:CLASS 21:CLASS 24:CLASS

fragments assigned reagent role:

containing 24

fragments assigned product role:

containing 12

fragments assigned reactant/reagent role:

containing 1

containing 5